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United States Environmental Protection Agency
Washington, DC 20460

ORIGINAL

| Document Description | Date |
| --- | --- |
| SAT P00-898 | 7/26/2000 |

[redacted]

[redacted]

Does not contain National Security Information (E.O. 12065)

[redacted]

[redacted]

EPA Form 7740-9 (rev. 10/92) Previous edition is obsolete

| STRUCTURE ACTIVITY TEAM REPORT ver. 04/98 [redacted] | |
|---|---|
| **Case #:** P-00-0898 | **DCN:** |
| **SAT Date:** 6/27/2000 | **SAT Chair:** L. Keifer |

**Submitter:** [redacted]

**Chemical Name:**

[redacted]

| **CAS RN:** [redacted] | **Trade Name:** [redacted] |
|---|---|

**Structure**

[redacted]

| | | |
|---|---|---|
| **Molecular Formula:** [redacted] | | |
| **Molecular Wt.** [redacted] | **WT%<500:** | **WT%<1000:** |
| **MP:** | **BP:** >500 | **Eq. Wt:** |
| **H2O Sol (g/L):** 1000 [redacted] | **V.P.** <0.000001 | |
| **Max. Prod. Volume (kg/yr):** [redacted] | **Physical State:** Solid (est) | |

**USE:**

Drilling additive [redacted]

| Related Case Numbers | Case Role | Related Case Numbers | Case Role |
|---|---|---|---|
| [redacted] | | [redacted] | |
| | | | |
| | | | |

| Focus | Date: JUL 6 2000 | Results: Focus Drop |
|---|---|---|

STRUCTURE ACTIVITY TEAM REPORT [redacted] 06/27/00

CASE NUMBER: **P00-0898**

RELATED CASES: [redacted] [redacted] [redacted]

CONCLUSIONS/DISCUSSIONS

| TYPE OF CONCERN: | HEALTH | ECOTOX |
|---|---|---|
| LEVEL OF CONCERN: | 1-2 | 2 |

KEYWORDS: REPRO NEURO
AQUATOX

SUMMARY OF ASSESSMENT

FATE: Solid, [redacted] analog
LogKow = -1.42(E); S (25°C) = 817 g/L(E); H < 1.00E-8(E)
MP (C) = 228(E); BP (C) > 400(E); VP @ 25C (mm) < 1.0E-6(E)
LogKoc = 2.99(E); LogBCF = 0.50(E);
POTW removal (%) = 90 via sorption; [redacted] is readily biodegradable (MITI database).
Time for complete ultimate aerobic biodeg = da-wk
PBT Potential: P1B1T1
Sorption to soils/sediments = moderate
*CEB FATE: Migration to ground water = negl - slow

HEALTH: Not absorbed from the skin, absorbed from the lung (pchem), absorbed from the GI tract (analog). Concern for reproductive toxicity based on [redacted] [redacted] [redacted] (2-generation reproductive toxicity test in rats with a NOEL of 150 mg/kg, LOEL = 500 mg/kg with decreased litter size and decreased post-natal weight gain) and neurotoxicity based on an acute study with [redacted] [redacted] tremors and ataxia at non-lethal doses, rat oral $LD_{50}$ = 830 mg/kg).

*CEB HEALTH: Low moderate concern (Inhalation)

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

| | | | |
|---|---|---|---|
| fish 96-h LC50 | = | 960.0 | P |
| fish (RT) 96-h LC50 | = | 3900.0 | M S,N |
| daphnid 48-h LC50 | = | 55.0 | P |
| green algal 96-h EC50 | = | 54.0 | P |
| fish chronic value | = | 100.0 | P |
| daphnid ChV | = | 6.0 | P |
| algal ChV | = | 7.8 | P |

Predictions are based on SARs for [redacted] [redacted]; SAR chemical class = [redacted] [redacted] [redacted]; log Kow for the free amine = 0.09 (ClogP); [redacted]; pH7; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <180.0 mg/L as CaCO3; and TOC <2.0 mg/L; moderate concern;

assessment factor = 10.0
concern concentration = 0.600
*CEB ECOTOX: All releases to surface waters.

SAT Co-chair: Leonard Keifer 260-1548

| NCSAB SAT REPORT | | CBI? (Y/N): |
|---|---|---|
| PMN: P-00-0898 | CAS RN: [redacted] | |
| Chemical Name: [redacted] | | Analogs: |
| | | PV: [redacted] |

Structure:

[redacted]

Use:
Drilling additive [redacted]

| | | | | | |
|---|---|---|---|---|---|
| Formula: [redacted] | | Eq Wt: | | | |
| MW: [redacted] | Wt%<500: | Wt%<1000 | | | |
| MP: | | BP: | >500 | VP: | <0.000001 |
| WS (g/L): 1000 | Physical State: | Solid (est) | Log P: 0.09 (CLOGP) | | |

| Endpoint (mg/L) | Est. Value | Meas. Value | Comments |
|---|---|---|---|
| Fish 96-h | 960 | | |
| Daphnid 48-h | 55 | | |
| Algal 96-h | 54 | | |
| Fish ChV | 96 | | |
| Daphnid ChV | 5.5 | | |
| Algal ChV | 7.8 | | |
| | | | |
| BCF | | | |

| | | | | | |
|---|---|---|---|---|---|
| CHEMICAL CLASS: | | | SAR: [redacted] | | |
| ECOTOX CONCERN | H | (M) | L | CONCERN CONCENTRATION | 0.55 |
| DATE: Monday June 19, 2000 | | | | ASSESSOR: | |

00 898

TOXICITY DATA SUMMARY (One page for each test)

PMN TYPE: P

PMN YEAR: 00 [redacted]

PMN NUMBER: 898

REVIEWER: JVN [redacted]

CHEMICAL CLASS: [redacted]

SPECIES TESTED : Common Name RT >36d [redacted]

Scientific

| TIME | EFFECT TYPE | CONCENTRATION (mg/L) |
|---|---|---|
| 24h | EC50 | 9500. |
| 48h | EC50 | 4800. |
| 72h | EC50 | 4400. |
| 96h | EC50 | 3900. |
| 24h | LC50 | 10,000. |
| 48h | LC50 | 4800. |
| 72h | LC50 | 4400. |
| 96h | LC50 | 3900. |
| 96h | EC10 | |
| 96h | EC90 | |
| 96h | NOEC | |
| 96h | LOEC LC30 | 3100. |
| 96h | GMATC | |
| 96h | LC100 | 6250. |
| 96h | EC100 | 6250. |
| 48h | EC10 | |
| 48h | EC90 | |
| 48h | NOEC | |
| 48h | LOEC | |
| 48h | GMATC | |
| 48h | LC100 | |
| 48h | EC100 | |
| | | |
| | | |
| | | |
| | | |

ACTIVE INGREDIENT: Convert all effect concentrations to 100% active ingredient.

DT 100% AI Unknown aeration pH 8.5 @ 50 g/L

REMARKS : P50% in H2O; S, N; FW, deq; pH 8.1; S 50 g ai/L pH 10.5 → 8.0; [redacted]

[redacted]

SMILES : [redacted]
CHEM :
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: [redacted]
MOL WT : [redacted]
Log Kow: 0.09 (User entered)
Melt Pt: 25.00 deg C
Wat Sol: 3.296E+005 mg/L (calculated)

ECOSAR v0.99e Class(es) Found
---
[redacted]

| ECOSAR Class | Organism | Duration | End Pt | Predicted mg/L (ppm) | MW adj |
|---|---|---|---|---|---|
| [redacted] (Baseline Toxicity) | : Fish | 14-day | LC50 | 7191.939 | |
| [redacted] | : Fish | 96-hr | LC50 | 534.117 | 960 |
| [redacted] | : Daphnid | 48-hr | LC50 | 30.809 | 55 |
| [redacted] | : Green Algae | 96-hr | EC50 | 30.073 | 54 |
| [redacted] | : Green Algae | 96-hr | ChV | 4.327 | 7.8 |

Note: * = asterick designates: Chemical may not be soluble enough to measure this predicted effect.
Fish and daphnid acute toxicity log Kow cutoff: none
Green algal EC50 toxicity log Kow cutoff: none
Chronic toxicity log Kow cutoff: none
MW cutoff: none

CHEMICAL: Unknown 10:45:29 06/26/:0

MOL WT : [redacted]

MOL FOR: [redacted]

SMILES : [redacted]

ISOC-ID: [redacted]

FRAG-ID: [redacted]

H-COUNT: [redacted]

| Class | Type | Contribution Description | Comment | Value |
|---|---|---|---|---|
| [redacted] | [redacted] | [redacted] | [redacted] | [redacted] |
| [redacted] | [redacted] | [redacted] | [redacted] | [redacted] |

Press ENTER to continue..

OPPT STRUCTURE ACTIVITY TEAM (SAT) MEETING DATE 7-11-00

| ATTENDEES | SIGNATURE |
|---|---|
| **CHEMISTRY** | |
| ✓ Paul Bickart | Paul Bickart |
| Diana Darling | |
| Rich Engler | |
| Greg Fritz | |
| Fred Metz | |
| Daniel Lin | |
| ✓ Kathy Schechter | Kathy Schechter |
| | |
| **ENVIRONMENTAL FATE** | |
| Bob Boethling | |
| David Lynch | |
| ✓ Gary Thom | gcthom |
| | |
| | |
| **HEALTH** | |
| Katherine Anitole | |
| ✓ Michael Cimino | Michael Cimino |
| Ilda McKenna | |
| Leonard Keifer | |
| ✓ David Lai | David Lai |
| ✓ Jim Murphy | Jim Murphy |
| ✓ Deborah Norris | D Norris |
| ✓ Ronald Ward | |
| Yin Tak Woo | |
| | |
| | |
| **ENVIRONMENTAL EFFECTS** | |
| ✓ Gordon Cash | Gordon Cash |
| Vince Nabholz | |
| Maggie Wilson | |
| | |
| **SAT CHAIRPERSON/OTHER** | |
| Rebecca Jones | |
| ✓ Leonard Keifer | L Keifer |
| Vince Nabholz | |
| | |
| Robert Morcock | |